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NUMERICAL STUDIES IN GAS DYNAMICS.(U)
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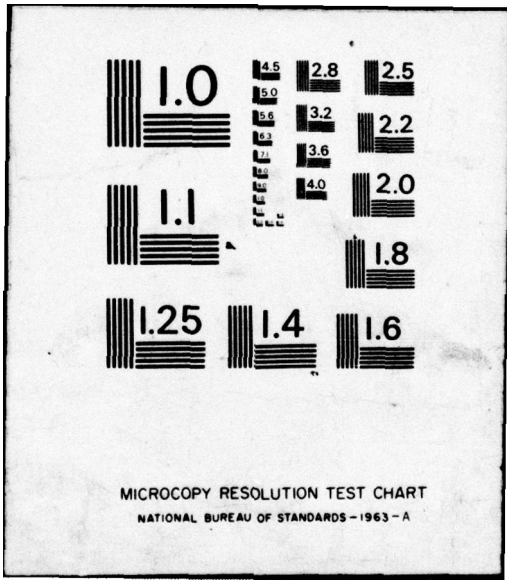
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FINAL SCIENTIFIC REPORT

RESEARCH GRANT AFOSR-72-2336

NUMERICAL STUDIES IN GAS DYNAMICS

Submitted to the

Air Force Office of Scientific Research

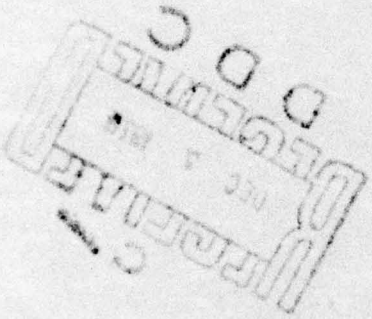
by the

Department of Aeronautical Engineering
University of Sydney
Sydney, N.S.W. Australia.

14th October, 1976.

Principal Investigator: G.A. Bird,
Professor of Aeronautical Engineering.

This document summarizes work supported by Grant AFOSR-72-2336 over the complete grant period April 15, 1972 to October 14, 1976 and describes the work carried out during the period from April 15, 1974.



1. REVIEW OVER COMPLETE GRANT PERIOD 1972-1976

1.1 Major Developments

Most of the research has been associated with the further development and application of the direct simulation Monte Carlo method for the modeling of gas flows at the molecular level. A monograph[1] which includes a full description of the method, together with a number of new applications, has been written and published during this period. Acknowledgment was made generally of the support provided by the AFOSR during the whole period over which the method has been developed and specifically to the current grant with respect to some new applications that appear in the book.

A significant development has been the demonstration that the computations are best carried out on a dedicated minicomputer rather than on a large machine in a computing center. The probability of this was proposed for preliminary investigation in 1973 and this led to a proposal to the Australian Research Grants Committee for a PDP 11/40 system. This submission was successful and the computer was installed early in 1975. Since this time, it has run twenty four hours a day and seven days a week without an operator and the improvement in cost-effectiveness has been found to be near two orders of magnitude. The reduction in computing costs has meant that small disturbance flows, which had previously been thought to be inaccessible to the method, can now be studied. The first demonstration of this capability was for the classical surface slip or Kramers problem[9]. The flow profile was studied at Mach numbers as low as 0.05, with the computer runs being sufficiently long to reduce the statistical scatter to one part in a thousand.

An additional consequence of the practicability of very long runs is that molecular simulation can now be considered is an alternative to finite difference methods for the computation of some continuum flows. This point was first demonstrated[4] by lengthy runs on a large computer and a more recent study[8] has further demonstrated the advantages of the dedicated minicomputer. The advantages of the molecular simulation over the finite difference continuum representation relate to the absence of stability problems and the ease of incorporation of complex flow boundaries. The molecular approach appears to be most advantageous for problems involving complex shock wave interactions, but having inviscid boundaries. On the other hand, the method has been used[5] to study a viscous problem at sufficiently low Knudsen number that the conclusions should be valid in continuum flow.

The most recent extension of the method has been to reacting gas flows. Particular attention has been paid to the dissociation-recombination reaction in a diatomic gas. The model permits the analytical determination of the equilibrium state[1] and it has now been applied to the reaction zone behind a strong shock wave. Specific cases have been computed

for nitrogen and the results have been compared with existing experimental data for nitrogen[10].

One topic, the study of the forces on very small suspended particles in the atmosphere started[3] as a simulation project, but led to a significant experimental study[6].

1.2 Publications

1 Bird, G.A. "Molecular Gas Dynamics", Oxford University Press, London, 1976.

2 Bird, G.A. "Impact of a Freely Expanding Gas on a Wall", Phys. Fluids, Vol. 16, 1973, p. 1830.

3 Tong, N.T. "Photophoretic Force in the Free Molecule and Transition Regimes", J. Colloid and Interface Sciences, Vol. 43, 1973, p. 78.

4 Bird, G.A. "Near Continuum Impact of an Underexpanded Jet Plume on a Wall", Proceedings of the First AIAA Computational Fluid Dynamics Conference", 1973, p. 103.

5 Bird, G.A. "The Nozzle Lip Problem", in "Rarefied Gas Dynamics" (ed. M. Becker and M. Fiebig), p. A 22-1, DFVLR Press, Porz-Wahn.

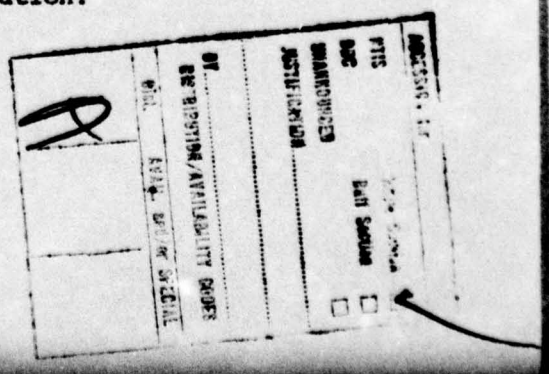
6 Tong, N.T. "Experiments on Photophoresis and Thermophoresis", J. Colloid and Interface Sciences, Vol. 51, 1975, p. 143.

7 Bird, G.A. "Collision Rates and Collisional Energy Distributions within Shock Waves", in "Modern Developments in Shock Tube Research", (Ed. G. Kamimoto), 1975.

8 Auld, D.J. and Bird, G.A. "The Transition from Regular to Mach Reflection", AIAA Paper 76-322, 1976.

9 Bird, G.A. "Direct Simulation of the Incompressible Kramers Problem", Proc. of Tenth International Symposium on Rarefied Gas Dynamics. To be published by AIAA.

10 Bird, G.A. "Direct Molecular Simulation of a Dissociating Diatomic Gas". Submitted for publication.



2. REPORT ON PERIOD 1975-1976.

The final extension of the Grant was from April 15, 1975 to April 14, 1976 but, due to a period of absence of the Principal Investigator, this was extended to October 14, 1976. Four topics were included in the proposal and the work done on each of these is described below.

2.1 Collision Rates and Collisional Energy Distribution within Shock Waves.

This work led to publication 7 in the list of Section 1.2. The direct simulation Monte Carlo method was used to determine the collision rate and the distribution of relative translational energy between colliding molecules within strong shock waves. The results were compared with the corresponding theoretical quantities in an equilibrium gas. The objective was to determine whether the region of marked translational nonequilibrium within the wave needs to be taken into account in the interpretation of reaction rate experiments in shock tubes. It was found that a correction should be applied to measured relaxation distances behind shock waves. The magnitude of this correction is of the order of ten times the translational shock thickness.

2.2 Calculations with Quantum Mechanics Cross-sections.

Dr. A.U. Chatwani of the Max-Planck Institut für Strömungsforschung spent six weeks in the Aeronautical Engineering Department and incorporated quantum theory collision cross-sections into the existing simulation program for a steady spherical expansion. This program had been used to study the onset of translational non-equilibrium, and this generally occurs at very low temperatures where quantum effects are significant. Dr. Chatwani continued the work after his return to Germany and carried out a thorough study of terminal Mach numbers, both for real gases and the idealised models. This work was presented at the Tenth International Symposium on Rarefied Gas Dynamics in a paper entitled "Monte Carlo Simulation of Nozzle Beam Expansions" and is to be published in the proceedings.

2.3 The Onset of Mach Reflection

The direct simulation Monte Carlo method was used to study the transition from regular to Mach reflection of oblique two-dimensional steady shock waves. Particular attention was paid to the region of Mach number and deflection angle in which both types of reflection are theoretically possible. The results indicated that regular reflection can occur in the region where both types of reflection are possible. The study confirmed that the molecular approach can provide a practical alternative to finite difference and finite element methods for the computation of some continuum flows, especially when a dedicated mini-computer is used instead of a large machine in a general computing center. A paper was presented at the AIAA 9th Fluid and Plasma Dynamics Conference.

2.4 The Dissociation-Recombination Reaction in a Shock Tube

The direct simulation Monte Carlo method has been extended to cover molecular dissociation and recombination reactions. The model also includes internal degrees of freedom with separate relaxation times for rotation and vibration. The model is based on a classical collision theory analysis that provides an expression for the equilibrium state and allows the appropriate simulation parameters to be inferred from thermodynamic data for real gases. The model was first tested by the computation of the constant volume relaxation of a homogeneous gas sample. A finite difference procedure was then used to extend this program to cover the dissociation relaxation zone behind strong normal shock waves. A number of nitrogen cases were computed and the results were in agreement with existing experimental data. A paper has been submitted to the Journal of Computational Physics.

In addition to the work on the above topics, the work on the incompressible Kramers problem (reference 9 in the list of Section 1.2) was carried out during this period.

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

A survey is made of the overall development of the direct simulation Monte Carlo method, ~~over the period 1972 to 1976.~~ This is a method for the computation of gas flows at the molecular level. The major advances have related to the extension of the method to cover some continuum flows, small disturbance flows and reacting gas flows. All these require very extensive computation and dedicated mini-computers have been shown to be one or two orders of magnitude more cost-effective than large general purpose machines in conventional computer centers.

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